valine and d-alanine take place below 270K, and they do not appear in l-equivalents. Recently, the phenomenon was investigated using differential scanning calorimetry and laser Raman spectroscopy [1]. It was also studied by X-ray diffraction (elementary cell against the temperature measurements) [2], and neutron diffraction (structure solution and refinement) [3]. These studies have questioned previous findings.

Because both diffraction methods do not consider subtle electronic effects, we have decided to apply experimental charge density methods to investigate these possible phase transitions. Here in this communication we present a comparison of charge densities of selected amino acids which have been not determined so far.

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Keywords: charge density, amino acids

MS90.P03

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Multi component crystals of active pharmaceuticals ingredients: 1,1-dimethylbiguanide hydrochloride, diflunisal and valproic acid

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The design of multi-component crystals requires knowledge of robust supramolecular synthon. We explore the applicability heterosynthons based on O-H···N and N-H···O hydrogen bonds for the synthesis of pharmaceutical multi-component crystals with three important pharmaceutical molecules: the anti-diabetic drug 1,1-dimethylbiguanide hydrochloride (1), the anticonvulsant drug valproic acid (2),the anti-inflammatory drug diflunisal (3). Both traditional solution co-crystallization and solvent-drop grinding co-crystallization have led to the discovery of 1,1-dimethylbiguanide-oxalate monohydrate salt(1:2.5), methylbenzylammonium-valproate salt (1:1) and diflunisal-hexamethylenetetramine (1:1) co-crystals. In the course of the experiments a new hydrate of succinic acid was obtained.

Keywords: co-crystallization, multi-component crystal, hydrogen bonding.

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Experimental charge density distribution in *N*-o-vanillylidene-L-histidine

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Charge density distribution in the crystal structure of *N*-o-vanillylidene-L-histidine (OVHIS) has been determined by using of a high-resolution, low-temperature, single-crystal X-ray diffraction data set. The Hansen-Coppens multipole model [1] was used to describe the electron density distribution in the OVHIS molecule. It was found that OVHIS exists in a double zwitterionic form. Four oxygen atoms in the molecule are approximately coplanar, carry significant negative charge and they together form an area of strong negative electrostatic potential. The OVHIS molecule is very polarized and has a high molecular dipole moment in solid state. A topological analysis of the total electron density, based on Bader's Quantum Theory of Atoms in Molecules (QTAIM) [2], confirmed the existence of 12 intermolecular interactions and corresponding (3,–1) bond critical points. It seems that intermolecular hydrogen bonds (especially two strong charge-assisted N–H···O bonds) significantly contribute to existing charge density distribution in the OVHIS molecule and its electrostatic properties.

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Keywords: zwitterion, charge density ditribution, electrostatic properties

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Rerefinement of tricyclic acyclovir: $C_{11}H_{13}N_5O_3{\cdot}2H_2O$

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Tricyclic acyclovir, 3-[(2-hydroxyethoxy)-methyl]-6-methyl-3*H*-imidazolo[1,2-*a*]purin-9(5*H*)-one, has been reported as the dihydrate, $C_{11}H_{13}N_5O_3{\cdot}2H_2O$. The complex concerted hydrogen bond network of water and tricyclic acyclovir molecules was suggested to be related to the solvation of the molecules in solution [1]. The $Z' = 2$ structure contains four independent solvent water molecules, forming an $(H_2O)_8$ cluster through a strong hydrogen bond (d[O···O] = 2.81 Å) between two water molecules across an inversion center. Three of the independent water molecules are ordered while the inversion center requires one hydrogen atom in the fourth to be statistically disordered. The second disordered hydrogen position is a strong donor to the hydroxyl group of the side chain of one independent molecule of tricyclic acyclovir. The hydroxyl group in turn relates to an equivalent group on the next molecule through a strong hydrogen bond (d[O···O] = 2.67 Å) across another inversion center requiring statistical disordering of the hydroxyl hydrogen atom [2]. The result of the hydrogen atom disorders is concerted chains propagating in opposite directions, which differ only in the placement of the hydrogen atoms.

The $(H_2O)_8$ clusters are essentially perpendicular to the chains and create a 2D network with both independent tricyclic acyclovir molecules, using strong O–H···O water-water and water-drug, and O–H···N water-drug interactions linking the entire structure into an extensive, strong 3D hydrogen bonded network. The supramolecular interactions of the disordered side chain disorder of tricyclic acyclovir provide a rationalization of the nonstatistical disorder previously reported [1] through clear C–H···O preferences for the major component at two atom sites, no clear preference at the ether oxygen atom site, and a weak C–H···O preference at one minor component site.